Calculation of Dynamic Heat Flow in Walls

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Introduction

Assessment of the energy balance of buildings depends on estimations of the temperature driven dynamic heat flow through walls between inside and outside. ISO 13790:2008-03-01 "Energy performance of buildings – Calculation of energy use for space heating and cooling" mentions different methods to calculate the dynamic heat transfer in walls at hourly changing temperatures.

In this work the Crank-Nicolson Method in combination with the Thomas algorithm is used to calculate dynamic heat transfer through walls.

Heat Flow Theory

The heat Q [J] transferred between two points at the temperature difference ΔT [K], is proportional to their distance x [m], surface area A [m^2], thermal conductivity λ [W/(m·K)] and duration of the flow Δt [s] (equation 1).

$$Q = \lambda \cdot A \cdot \frac{\Delta T}{x} \cdot \Delta t \quad [J] \tag{1}$$

Q : heat [J]
λ : thermal conductivity [W/(m·K)]
A : surface area [m^2]
ΔT : temperature difference [K]
Δt : duration of the heat transfer [s]
x : distance between the two places where the heat transfer occurs [m],

The heat flow $\dot{Q}$ [W] is the heat transferred per unit of time:

$$\dot{Q} = \frac{Q}{\Delta t} = \lambda \cdot A \cdot \frac{\Delta T}{x} \quad [W] \tag{2}$$

$\dot{Q}$: heat flow [W = J/s]

If the temperature difference changes in time, the heat flow becomes dynamic and changes as well. The dynamic heat flow depends on the heat capacity of the material.

Example:

A cup of hot coffee gets colder in time because of the temperature difference between coffee and the surrounding air. When the coffee has reached air temperature, ΔT [K] becomes zero and the heat flow stops. The time, in which the coffee reaches the surrounding air temperature is depending on the heat content Q [J] of the coffee. The heat content is proportional to the specific heat capacity c_m [J/(kg·K)] and Temperature T [K] of the coffee (see equation 3).

$$Q = c_m \cdot \rho \cdot T \cdot V \qquad [J] \tag{3}$$

Q : heat content [J]
c_m : specific heat capacity [J/(kg·K)]
ρ : density [kg/m³]
T : temperature [K]
V : volume [m³]

Calculation of dynamic heat flow with the Crank-Nicolson method

The Crank-Nicolson method is a finite difference method that can be used to calculate the dynamic heat flow numerically. This shall be demonstrated below.

We assume there are 3 elements [i-1], [i] and [i+1] with equal thickness x [m]. Each element contains a certain amount of heat Q [J] and the heat is concentrated in the centre (see figure 1). At the specific time [j]:

- element [i-1] is at temperature $T_{i-1,j}$,
- element [i] is at temperature $T_{i,j}$ and
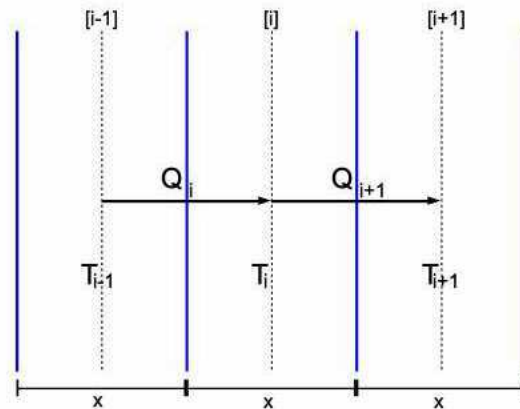- element [i+1] is at temperature $T_{i+1,j}$.

Figure 1: Schematic view of the heat flow between three elements with thickness x

In the duration Δt [s] the heat Q_i [J] flows from element [i-1] to element [i] and the heat Q_{i+1} [J] flows from element [i] to element [i+1]:

$$Q_i = \lambda \cdot \frac{T_{i-1} - T_i}{x} \cdot A \cdot \Delta t \qquad [J]$$

$$Q_{i+1} = \lambda \cdot \frac{T_i - T_{i+1}}{x} \cdot A \cdot \Delta t \qquad [J]$$

After a duration Δt at the time [j+1]:

- element [i-1] is at temperature $T_{i-1,j+1}$,
- element [i] is at temperature $T_{i,j+1}$ and
- element [i+1] is at temperature $T_{i+1,j+1}$.

The Crank-Nicolson method assumes that the heat flow during the duration Δt is the static mean heat flow between the heat flow at time [j] and that at time [j+1]:

$$\dot{Q}_i = \frac{\dot{Q}_{i,j} + \dot{Q}_{i,j+1}}{2} \qquad [W] \tag{4}$$

$$\dot{Q}_{i+1} = \frac{\dot{Q}_{i+1,j} + \dot{Q}_{i+1,j+1}}{2} \qquad [W] \tag{5}$$

In this time the heat content of element [i] changes by ΔQ [J], when the incoming heat flow and the outgoing heat flow differ:

$$\Delta Q_i = (\dot{Q}_i - \dot{Q}_{i+1}) \cdot \Delta t$$

Using equations (4) and (5) for Q_i and Q_{i+1}:

$$\Delta Q_i = \lambda \cdot A \cdot \left[T_{i-1,j} - 2T_{i,j} + T_{i-1,j+1} - 2T_{i,j+1} + T_{i+1,j} + T_{i+1,j+1} \right] \cdot \frac{\Delta t}{2 \cdot x}$$

According to equation (3), the change in the heat content ΔQ_i [J] of element [i] is dependent on the heat capacity c_m [J/(kg·K)]:

$$\Delta Q_i = c_m \cdot \rho \cdot (T_{i,j+1} - T_{i,j}) \cdot A \cdot x$$

This leads to:

$$\frac{1}{2} \cdot \frac{\lambda \cdot \Delta t}{c_m \cdot \rho \cdot x^2} \left[T_{i-1,j} - 2 \cdot T_{i,j} + T_{i-1,j+1} - 2 \cdot T_{i,j+1} + T_{i+1,j} + T_{i+1,j+1} \right] = (T_{i,j+1} - T_{i,j})$$

With $r = \frac{\lambda \cdot \Delta t}{c_m \cdot \rho \cdot x^2}$ being called the <u>modem</u>, this transforms to:

$$\left[r \cdot T_{i-1,j} - 2 \cdot r \cdot T_{i,j} + r \cdot T_{i-1,j+1} - 2 \cdot r \cdot T_{i,j+1} + r \cdot T_{i+1,j} + r \cdot T_{i+1,j+1} \right] = (2 \cdot T_{i,j+1} - 2T_{i,j})$$

Which can be written as equation (6):

$$(2 + 2 \cdot r) \, T_{i,j+1} = r \cdot T_{i-1,j} + r \cdot T_{i-1,j+1} + r \cdot T_{i+1,j} + r \cdot T_{i+1,j+1} + (2 - 2 \cdot r) T_{i,j} \tag{6}$$

This equation states, that the temperature of element [i] can be calculated at time [j+1], once the temperatures of elements [i-1], [i] and [i+1] are known at time [j] and the temperatures of elements [i-1] and [i+1] are known at time [j+1] (see table 1).

Time	Element		
	[i-1]	**[i]**	**[i+1]**
[j]	$T_{i-1,j}$ known primary definition	$T_{i,j}$ known primary definition	$T_{i+1,j}$ known primary definition
[j+1]	$T_{i-1,j+1}$ known boundary condition	$T_{i,j+1}$ unknown to calculate	$T_{i+1,j+1}$ known boundary condition

Table 1: Definition of the temperature values T

The definition of the temperature values at time [j]=1 is called <u>primary definition</u>. The values for T [°C] in the boundary elements [i-1] and [i+1] are called <u>boundary conditions</u>.

Calculation of the dynamic heat flow through more than 3 elements

To calculate dynamic heat flow through a wall, this wall needs to be divided into n elements of thickness x [m] perpendicular to the heat flow.
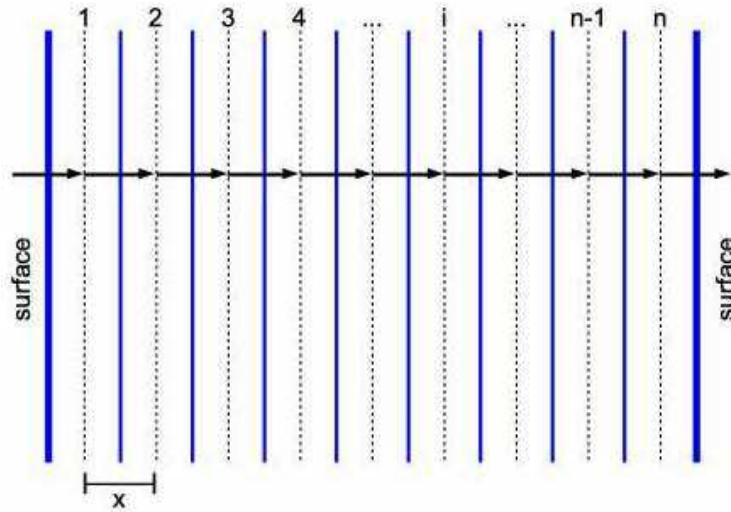

Figure 2: Partitioning of a system of n elements of thickness x and the heat flow through them ($T_1 > T_n$)

If there are more than 3 elements (1 < i < n), $T_{i,j+1}$ cannot be calculated the same way as shown by equation (6) as the temperatures $T_{2,j+1}$ to $T_{n-1,j+1}$ are unknown and only the boundary conditions $T_{1,j+1}$ and $T_{n,j+1}$ are known (see table 2).

Time	Element [i]						
	[1]	**[2]**	**...**	**[i]**	**...**	**[n-1]**	**[n]**
[j]	$T_{1,j}$ known prim. def.	$T_{2,j}$ known prim. def.	**...**	$T_{i,j}$ known prim. def.	**...**	$T_{n-1,j}$ known prim. def.	$T_{n,j}$ known prim. def.
[j+1]	$T_{1,j+1}$ known bound. cond.	$T_{2,j+1}$ unknown **to calc.**	**...**	$T_{i,j+1}$ unknown **to calc.**	**...**	$T_{n-1,j+1}$ unknown **to calc.**	$T_{n,j+1}$ known bound. cond.

Table 2: Definition of the temperature values T for a wall with n elements

Equation (6) is rewritten as equation (7) with the temperatures at time [j+1] on the left-hand side and the temperatures at time [j] on the right-hand side.

$$-r \cdot T_{i-1,j+1} + (2 + 2 \cdot r) \cdot T_{i,j+1} - r \cdot T_{i+1,j+1} = r \cdot T_{i-1,j} + (2 - 2 \cdot r) \cdot T_{i,j} + r \cdot T_{i+1,j} \quad (7)$$

As the temperatures on the right-hand side of equation (7) are known, this is a tridiagonal problem which can be solved with the tridiagonal matrix algorithm (Thomas algorithm). Thus, the unknown temperatures on the left-hand side of equation (7) can be calculated.

Equation (7) is rewritten as:

$$d_i = a \cdot T_{i-1,j} + b \cdot T_{i,j} + c \cdot T_{i+1,j} \tag{8}$$

With

$$a = r$$

$$b = 2 - 2 \cdot r$$

$$c = r$$

In matrix notation:

$$\begin{bmatrix} a & b & c & 0 & & 0 \\ 0 & a & b & c & & \\ & & \ddots & \ddots & \ddots & \\ 0 & & & a & b & c \end{bmatrix} \cdot \begin{bmatrix} T_{1,j} \\ T_{2,j} \\ T_{3,j} \\ \vdots \\ T_{n-1,j} \\ T_{n,j} \end{bmatrix} = \begin{bmatrix} d_2 \\ d_3 \\ \vdots \\ d_{n-1} \end{bmatrix}$$

This tridiagonal matrix is of size $[n \times (n-2)]$ as the temperatures $T_{1,j+1}$ and $T_{n,j+1}$ in the boundary layers (first and last layers of the wall) are known for time [j+1] and the temperatures from $T_{2,j+1}$ to $T_{n-1,j+1}$ need to be calculated.

The left-hand side of equation (8) can be written as:

$$d_i = -A \cdot T_{i-1,j+1} + B \cdot T_{i,j+1} - C \cdot T_{i+1,j+1} \tag{9}$$

With

$$A = r$$

$$B = 2 + 2 \cdot r$$

$$C = r$$

In order to calculate the temperatures $T_{i,j+1}$ a linear dependency from $T_{i-1,j+1}$ is used:

$$T_{i-1,j+1} = e_{i-1,j+1} \cdot T_{i,j+1} + f_{i-1,j+1} \tag{10}$$

$$T_{i,j+1} = e_{i,j+1} \cdot T_{i+1,j+1} + f_{i,j+1} \tag{11}$$

Using equation (10) to substitute $T_{i-1,j+1}$ in equation (9) leads to:

$$d_i = -A \cdot (e_{i-1,j+1} \cdot T_{i,j+1} + f_{i-1,j+1}) + B \cdot T_{i,j+1} - C \cdot T_{i+1,j+1}$$

$$\Leftrightarrow T_{i,j+1} = T_{i+1,j+1} \cdot \frac{C}{B - A \cdot e_{i-1,j+1}} + \frac{d_i + A \cdot f_{i-1,j+1}}{B - A \cdot e_{i-1,j+1}} \tag{12}$$

Comparing equations (11) and (12) yields in expressions for the factor $e_{i,j+1}$ and constant $f_{i,j+1}$:

$$e_{i,j+1} = \frac{C}{B - A \cdot e_{i-1,j+1}} \tag{13}$$

$$f_{i,j+1} = \frac{d_i + A \cdot f_{i-1,j+1}}{B - A \cdot e_{i-1,j+1}} \tag{14}$$

Solving the tridiagonal problem for the new temperatures at time [j+1] starts with a forward sweep (from i=1 to i=n) modifying the constants $e_{i,j+1}$ and $f_{i,j+1}$ beginning with $e_{1,j+1} = 0$ and $f_{1,j+1} = T_{1,j+1}$ for the set boundary condition in element [1]. The solution is then obtained by back substitution (from i=n-1 to i=2) according to equation (11), starting with the boundary conditions in element n.

The Crank-Nicolson algorithm might start to oscillate if the temperature differences are too high. It is therefore important, to keep an eye on the modem r. The system is stable when r has values smaller than 1. This can be reached as Δt and x are chosen accordingly. For the use of this algorithm for walls, a thickness of the elements of $x = 0{,}01$ m and $\Delta t = 60$ s are appropriate and stable. To reduce the calculation time, Δt can be increased to 300 s if the differences between $T_{i-1,j}$, $T_{i,j}$ and $T_{i+1,j}$ are not too big and the system does not oscillate.

Example for calculation in Python

The Python code CRANK_01.py (version 2020.07.05) is an example to calculate the temperature change in a wall of cellular concrete with 0.2m thickness in time steps of 60 seconds, when the temperature on one side decreases from 20°C to 0°C. The elements have a thickness of 0.01 m and the wall is virtually divided in 20 elements. The code contains an output command where the temperatures in the first and last 4 elements i[0], i[1], i[2], i[3], i[16], i[17], i[18], i[19] are printed for each time step. The first lines are important to control whether the system is oscillating or not.

Note:
If the time step is changed to 300 seconds in the code the system will oscillate until the 10th minute.

Steady state is reached when the temperature differences between all layers are the same. In the example this is at minute 1402 where the temperature of the element i[1] is stable at 18.9°C to one decimal place. The time to reach the steady state depends on the accuracy. One digit after the decimal point is suitable for walls, as the temperature is usually measured with an accuracy of +/- 0.1 °C.

Dynamic heat flow through two materials

Usually a wall consists of more than one material with different thermal conductivities and heat capacities. The heat flow between two different materials cannot be calculated by equations derived from equation (7). The problem can be solved by introducing two dummy elements D_1 and D_2 between the two layers of different materials and by the following assumptions:
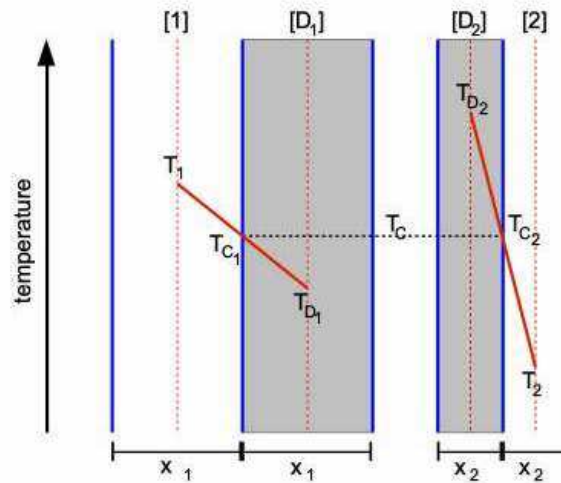

Figure 3: Introduction of two dummy elements between element [1] and element [2] of different thermal conductivities and different element widths x_1 and x_2. T_C is the contact temperature of the two elements on their common surface.

1.) The dummy elements have the same thickness and thermal conductivity as their adjoining elements.
2.) The contact temperature T_{C1} between the element and its dummy element is the mean value of the temperatures T_1 in the element [1] and the temperature T_{D1} of the respective dummy element [D1]. The same applies for the element [2] with the dummy element [D2].
3.) We assume that T_C is the same for both elements [1] and [2]: $(T_C = T_{C1} = T_{C2})$ and write equation 15:

$$T_C = \frac{T_1 + T_{D1}}{2} = \frac{T_2 + T_{D2}}{2} \quad \Rightarrow \quad T_{D1} = T_2 + T_{D2} - T_1 \tag{15}$$

4.) Further we assume that the heat flow density from element [1] to its dummy element [D1] is the same as the heat flow density received by element [2] from its dummy element [D2]:

$$\lambda_1 \cdot \frac{T_1 - T_{D1}}{x_1} = \lambda_2 \cdot \frac{T_{D2} - T_2}{x_2} \quad \Longleftrightarrow \quad \frac{\lambda_1 \cdot x_2}{\lambda_2 \cdot x_1} \cdot (T_1 - T_{D1}) = T_{D2} - T_2 \tag{16}$$

Substituting T_{D1} from equation (16) with equation (15) results in:

$$\frac{\lambda_1 \cdot x_2}{\lambda_2 \cdot x_1} \cdot [\, T_1 - (T_2 + T_{D2} - T_1)] = T_{D2} - T_2 \tag{17}$$

$$\frac{\lambda_1 \cdot x_2}{\lambda_2 \cdot x_1} = K \tag{18}$$

K is called the <u>coupling factor</u>. Introducing K to equation (17) yields an expression for the temperature T_{D2} on the dummy element [D2] on "left side" of element [2] in figure 3:

$$T_{D2} = \frac{2 \cdot K \cdot T_1 + (1 - K) \cdot T_2}{1 + K}$$

Generalized, K_1 is the coupling factor between the element [i-1] and the element [i] (see equation 19):

$$T_{D(i)} = \frac{2 \cdot K_1 \cdot T_{i-1} + (1 - K_1) \cdot T_i}{1 + K_1} \tag{19}$$

When the thermal conductivities λ and widths x of elements [i-1] and [i] are the same, the coupling factor K_1 between element [i-1] and element [i] will become $K_1 = \frac{\lambda_{i-1} \cdot x_i}{\lambda_i \cdot x_{i-1}} = 1$.

When the tridiagonal matrix algorithm sweeps through the elements [i+1] to element [i], the element composition will change on the "right" side of element [i] (see figure 3). We rename the dummy element "left" of element [i] to [D$_{left}$] and introduce another dummy element on the "right" side of element [i] as [D$_{right}$]. The temperature of the dummy element [D$_{right}$] can be calculated by substituting $T_{D(i)}$ in equation (19) with $T_{D(right)}$

$$T_{D(right)} = \frac{2 \cdot K_1 \cdot T_{i-1} + (1 - K_1) \cdot T_i}{1 + K_1} \tag{20}$$

To calculate $T_{D(left)}$ we use equation (15) and replace T_{D2} with $T_{D(left)}$. This leads to equation (21):

$$T_{D(left)} = \frac{2 \cdot T_{i+1} - (1 - K_2) \cdot T_i}{1 + K_2} \tag{21}$$

In This case the coupling factors are given by equation (22) and (23).

$$K_1 = \frac{\lambda_{i-1} \cdot x_i}{\lambda_i \cdot x_{i-1}} \qquad \text{for the "left" side of element [i]} \tag{22}$$

$$K_2 = \frac{\lambda_i \cdot x_{i+1}}{\lambda_{i+1} \cdot x_i} \qquad \text{for the "right" side of element [i]} \tag{23}$$

As the dummy temperatures are a substitution for the temperatures of the neighboring elements of element [i], those temperatures can be introduced to the left side of equation (7):

$$d_i = -r \cdot T_{i-1,j+1} + (2 + 2r) \cdot T_{i,j+1} - r \cdot T_{i+1,j+1}$$

$$d_i = -r \cdot (T_{D(left),j+1}) + (2 + 2r) \cdot T_{i,j+1} - r \cdot (T_{D(right),j+1})$$

$$d_i = -r \cdot \left[\frac{2 \cdot K_1 \cdot T_{i-1,j+1} + (1 - K_1) \cdot T_{i,j+1}}{1 + K_1} \right] + (2 + 2r) \cdot T_{i,j+1} - r \cdot \left[\frac{2 \cdot T_{i+1,j+1} - (1 - K_2) \cdot T_{i,j+1}}{1 + K_2} \right] \tag{22}$$

We introduce two new factors:

$$G_1 = r \cdot \frac{1 - K_1}{1 + K_1} \qquad \text{for the "left" side of element [i]} \tag{25}$$

$$G_2 = r \cdot \frac{1 - K_2}{1 + K_2} \qquad \text{for the "right" side of element [i]} \tag{26}$$

After mathematical transformations, d_i can be expressed from equation (24) as:

$$d_i = -(r - G_1) \cdot T_{i-1,j+1} + (2 + 2r - G_1 + G_2) \cdot T_{i,j+1} - (r + G_2) \cdot T_{i+1,j+1} \qquad (27)$$

Or identical to equation (9) as:

$$d_i = -A \cdot T_{i-1,j+1} + B \cdot T_{i,j+1} - C \cdot T_{i+1,j+1} \qquad (28)$$

With new constants A, B and C:

$$A = r - G_1 \qquad (29)$$

$$B = 2 + 2 \cdot r - G_1 + G_2 \qquad (30)$$

$$C = r + G_2 \qquad (31)$$

In order to calculate the factor $e_{i,j+1}$ and constant $f_{i,j+1}$ from the calculation of d_i at time [j] from the right side of equation (7), this side needs to be altered as well, introducing the dummy temperatures. This is done analogous to the left side shown above and yields in a similar expression:

$$d_i = A \cdot T_{i-1,j} + (2 - 2 \cdot r + G_1 - G_2) \cdot T_{i,j} + C \cdot T_{i+1,j} \qquad (32)$$

Solving the tridiagonal problem for elements with different thicknesses x and thermal conductivities λ at time [j+1] computing starts with a forward sweep from element [1] to [n], modifying the constants $e_{i,j+1}$ and $f_{i,j+1}$ beginning with $e_{1,j+1} = 0$ and $f_{1,j+1} = T_{1,j+1}$ for the set boundary condition in element [1]. In order to do this the constants r, K_1, K_2, G_1, G_2, A, B and C need to be computed. The solution is then obtained by back substitution from element [n-1] to [2] according to equation (11), starting with the boundary conditions in element [n].

When all "new" temperatures at the time [j+1] in all elements [2] to [n-1] are known, the heat flow Q_i between two elements during Δt can be calculated with equation (33) derived from equation (1).

$$Q_i = \frac{T_{(i,j+1)} - T_{(i+1,j+1)}}{\frac{x_i}{2 \cdot \lambda_i} + \frac{x_{i+1}}{2 \cdot \lambda_{i+1}}} \cdot A \cdot \Delta t \quad [J] \qquad (33)$$

Or as heat flow density q in [W/m²]

$$q_i = \frac{T_{(i,j+1)} - T_{(i+1,j+1)}}{\frac{x_i}{2 \cdot \lambda_i} + \frac{x_{i+1}}{2 \cdot \lambda_{i+1}}} \quad [\frac{W}{m^2}] \qquad (34)$$

Example 2

The Python code CRANK_02.py (version 2020.07.05) is an example to calculate the temperature change in a wall consisting of two different materials in time steps of 60 seconds. The wall consists of 0.2 m cellular concrete, 0.05 m expanded polystyrene (EPS) and is virtually divided into 25 elements of 0.01 m thickness. The temperature in the element i[n-1] decreases from 20 °C to 0 °C.

The output command prints the temperatures in the first and last 4 elements i[0], i[1], i[2], i[3], i[16], i[17], i[18], i[19] and the heat flows between the elements i[0]-i[1], i[1]-i[2], i[2]-i[3], i[3]-i[4], i[20]-i[21], i[21]-i[22], i[22]-i[23] and i[23]-i[24].

The steady state is reached at minute 5232 with the heat flow density of q = 7.99 W/m^2.

According to the heat equation it is expected that the steady state heat flow q is

$$q = \frac{\Delta T}{\frac{d_1}{\lambda_1}+\frac{d_2}{\lambda_2}} = \frac{20}{\frac{0,20}{0.160}+\frac{0.05}{0.035}} = 7.47 \quad \frac{W}{m^2}$$

q: Heat flow density [W/m2]
λ: Thermal conductivity [W/(ṁ·K)]
d: Thickness of the material [m]
ΔT: Temperature difference [°C]

The dynamic calculation in CRANK_02.py starts in the centre of the first element and ends in the centre of the last element. This results in an effective thickness of the cellular concrete part of 0.195m and the EPS part of 0.045m. Calculation with these values gives:

$$q = \frac{20}{\frac{0,195}{0.160}+\frac{0.045}{0.035}} = 7.99 \quad \frac{W}{m^2}$$

This is corresponding with the calculated dynamic heat flow in the steady state situation.

The heat flow is calculated with two places behind the decimal point, because the thermal conductivities of building materials as well as the U-values are given with an accuracy of two decimals.

It is recommended to check when the steady state heat flow is reached and to compare its value with the result of the static heat equation.

In another paper we will address the differences between the real thicknesses of the materials and the thicknesses used in calculations according to the Crank-Nicolson algorithm. There we will also focus on the boundary conditions of the materials in thermal contact with fluid media like air.